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Inventor
search:
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10/088425

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NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
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NEWS 15	Jul 30	NETFIRST to be removed from STN
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NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
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NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
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NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 27	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985

NEWS EXPRESS	October 14 CURRENT WINDOWS VERSION IS V6.01, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
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E3           19 --> TAKASE MITSURU/AU
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E23          37      TAKASE NOBUMITSU/AU
E24           9      TAKASE NOBUO/AU
E25           1      TAKASE NOBUTAKE/AU

=> S (E3) AND (CARBOXAMID?)
            19 "TAKASE MITSURU"/AU
         16882 CARBOXAMID?
L15           2 ("TAKASE MITSURU"/AU) AND (CARBOXAMID?)

=> s l15 not l9
L16           1 L15 NOT L9

=> d l16 ibib abs hitstr
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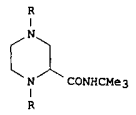
L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:120860 CAPLUS
DOCUMENT NUMBER: 132:180586
TITLE: Method for preparation of piperazine-2-**carboxamide** derivatives
INVENTOR(S): Hirai, Yukio; **Takase, Mitsuru**; Takata, Mitsumasa; Nagasaki, Fumihiko
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000053656	A2	20000222	JP 1998-238001	19980810

OTHER SOURCE(S): CASREACT 132:180586; MARPAT 132:180586
GI



I

AB The title compds. [I; R = H, Bn (benzyl)] are prepd. by cyclocondensation of N-tert-butyl-3-halo-2-hydroxypropanamide [XCH2CH(OH)CONHCMe3] with N,N'-dibenzylethylenediamine (BnNHCH2CH2NHBn). This process neither uses expensive platinum oxide nor specialized app. and gives N-tert-butyl-2-piperazinecarboxamide in good yields in an industrially advantageous manner, which is useful as an intermediate for drugs or agrochems. Thus, epoxidn. of N-tert-butylacrylamide with m-chloroperbenzoic acid in CHCl3 at room temp. for 100 h gave 58.0% N-tert-butyl-2,3-epoxypropanamide which was dissolved in CHCl3 and treated with concd. HCl at room temp. for 30 min to quant. give N-tert-butyl-3-chloro-2-hydroxypropanamide. Mesylation of the latter compd. with methanesulfonyl chloride in the presence of Et3N at room temp. for 1 h gave 72.6% N-tert-butyl-3-chloro-2-(methanesulfonyloxy)propanamide which underwent cyclocondensation with N,N'-dibenzylethylenediamine in the

L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS (Continued)
presence of DBU under reflux for 5 h to give 83.2% N-tert-butyl-1,4-dibenzyl-2-piperazinecarboxamide, I (R = Bn) and 10.5% CH2:CH(OSO2Me)CONHCMe3.

```
=> E YAMAZAKI SATORU/AU 25
E1            3     YAMAZAKI SATOKO/AU
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=> S (E3) AND (CARBOXAMID?)
            81 "YAMAZAKI SATORU"/AU
         16882 CARBOXAMID?
L17          2 ("YAMAZAKI SATORU"/AU) AND (CARBOXAMID?)

=> s l17 not l9
L18          1 L17 NOT L9

=> s l18 not l10
L19          1 L18 NOT L10

=> s l19 not l12
L20          1 L19 NOT L12

=> d l20 ibib abs hitstr
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L20 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:420276 CAPLUS
DOCUMENT NUMBER: 127:130827
TITLE: KMD-3213, a novel .alpha.1A-adrenoceptor antagonist, potently inhibits the functional .alpha.1-adrenoceptor in human prostate
AUTHOR(S): Moriyama, Nobuo; Akiyama, Katsuyoshi; Murata, Satoshi; Taniguchi, Jun; Ishida, Norio; **Yamazaki, Satoru**; Kawabe, Kazuki
CORPORATE SOURCE: Department of Urology, Faculty of Medicine, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113, Japan
SOURCE: European Journal of Pharmacology (1997), 331(1), 39-42
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB KMD-3213, (-)-(R)-1-(3-hydroxypropyl)-5-[2-[[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl]amino]propyl]indoline-7-**carboxamide**, is a novel and selective .alpha.1A-adrenoceptor antagonist. The potency of this drug to antagonize functional .alpha.1-adrenoceptor-mediated contraction in human prostatic smooth muscle was evaluated and compared with that of other .alpha.1-adrenoceptor antagonists. KMD-3213 inhibited noradrenaline-induced contractions with an apparent pKB value of 9.45, indicating a potency similar to that of tamsulosin. The affinity of prazosin for prostatic .alpha.1-adrenoceptors is given as potency for the .alpha.1L-adrenoceptor with an estd. pA2 value of 8.84. The data obtained in this study suggest that KMD-3213, an .alpha.1A-adrenoceptor-selective antagonist, has strong affinity for the .alpha.1L-adrenoceptor in the human prostate.

```
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E2            1     ISHII YUSUNOBU/AU
E3           87 --> ISHII YUTAKA/AU
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E13          12     ISHII ZENSHO/AU
E14           1     ISHIIA C/AU
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E24           8     ISHIIE TATSUJI/AU
E25           1     ISHIIGAME M/AU

=> S (E3) AND (CARBOXAMID?)
            87 "ISHII YUTAKA"/AU
         16882 CARBOXAMID?
L21          1 ("ISHII YUTAKA"/AU) AND (CARBOXAMID?)

=> d l21 ibib abs hitstr
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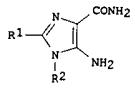
L21 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:228862 CAPLUS
DOCUMENT NUMBER: 134:252338
TITLE: Processes for the preparation of 4(5)-amino-5(4)-**carboxamidoimidazoles** and intermediates thereof
INVENTOR(S): Shibasaki, Hiroaki; Nagasaki, Fumihiko; Takase, Mitsuru; Yamazaki, Satoru; **Ishii, Yutaka**; Oohata, Kimihiko
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan; Ibaraki Kasei Co., Ltd.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001021592	A1	20010329	WO 2000-JP6397	20000920
W: CN, IN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2001151760	A2	20010605	JP 1999-330103	19991119
JP 2001302609	A2	20011031	JP 2000-116218	20000418
JP 2001158776	A2	20010612	JP 2000-284780	20000920
EP 1215206	A1	20020619	EP 2000-961096	20000920
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				

PRIORITY APPLN. INFO.:
JP 1999-264818 A 19990920
JP 1999-330103 A 19991119
JP 2000-116218 A 20000418
WO 2000-JP6397 W 20000920

OTHER SOURCE(S): CASREACT 134:252338; MARPAT 134:252338
GI



I

AB The invention provides novel processes for prepg. efficiently compds. of general formula (I) (wherein R1 and R2 are each independently hydrogen, optionally substituted C1-10 alkyl, C3-14 hydrocarbyl bearing an alicyclic skeleton, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted heterocyclyl, optionally substituted heterocyclylalkyl, N-optionally substituted carbamoyl, or alkoxycarbonyl) and intermediates thereof. Compds. of general formula I can be prepd. by subjecting compds. of general formula R2NHC(R1):NC(CN):C(NH2)CN (II; R1 and R2 are defined above) and/or salts thereof to cyclization hydrolysis in an aq. basic soln. Further, compds. of general formula II can be prepd. from industrially easily available diaminomaleonitrile in a high yield. The compds. I are useful as intermediates for agrochems. and drugs, e.g. dacarbazine and temozoromide (anticancer agent) and urazamide (liver-protective agent). Thus, 50 mL H2O and 43.0 g 25% NaOH were added to 8.0 g N-(2-amino-1,2-dicyanovinyl)formamidine and refluxed for 2 h, cooled to room temp., neutralized with 35% HCl to pH 7, concd. to dryness, treated with ethanol, and filtered for removing the insol. salt. The filtrate was treated with activated charcoal, filtered, and concd. to give a soln. of 4(5)-aminoimidazole-5-**carboxamide** (III) which was adjusted to pH .ltoreq.3 and cooled at .ltoreq.10.degree.. The pptd. crystals were collected by filtration and dried to give 84% III.HCl.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> E OOHATA KIMIHIKO/AU 25
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E25           6     OOHATA NOBUTAKA/AU

=> S (E3 OR E4) AND (CARBOXAMID?)
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              2 "OOHATA KIMIO"/AU
          16882 CARBOXAMID?
L22           1 ("OOHATA KIMIHIKO"/AU OR "OOHATA KIMIO"/AU) AND (CARBOXAMID?)

=> s l22 not l9
L23           0 L22 NOT L9

=> log y
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                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   52.69     342.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -5.58      -5.58

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NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
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NEWS 26	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 27	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985

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FILE 'HOME' ENTERED AT 15:57:19 ON 16 OCT 2002

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 OCT 2002 HIGHEST RN 461638-40-4
DICTIONARY FILE UPDATES: 15 OCT 2002 HIGHEST RN 461638-40-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L1 STRUCTURE UPLOADED

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FULL SCREEN SEARCH COMPLETED - 2532 TO ITERATE

100.0% PROCESSED 2532 ITERATIONS 560 ANSWERS
SEARCH TIME: 00.00.01

L2 560 SEA SSS FUL L1

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Uploading 100884251.str

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SEARCH TIME: 00.00.01

L4           89 SEA SSS FUL L3

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                                                 ENTRY    SESSION
FULL ESTIMATED COST                             281.32     281.53

FILE 'CAPLUS' ENTERED AT 15:59:33 ON 16 OCT 2002
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FILE LAST UPDATED: 15 Oct 2002  (20021015/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

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information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> s l2/p
L5          302 L2/P

=> d his

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     FILE 'REGISTRY' ENTERED AT 15:57:26 ON 16 OCT 2002
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L3              STRUCTURE UPLOADED
L4            89 S L3 FUL

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L5           302 S L2/P

=> s l5 and l4
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             35 L4
L6            4 L5 AND L4

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L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:228862 CAPLUS
DOCUMENT NUMBER: 134:252338
TITLE: Processes for the preparation of 4(5)-amino-5(4)-carboxamidoimidazoles and intermediates thereof
INVENTOR(S): Shibasaki, Hiroaki; Nagasaki, Fumihiko; Takase, Mitsuru; Yamazaki, Satoru; Ishii, Yutaka; Oohata, Kimihiko
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan; Ibaraki Kasei Co., Ltd.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001021592	A1	20010329	WO 2000-JP6397	20000920
W: CN, IN, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2001151760	A2	20010605	JP 1999-330103	19991119
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JP 2001158776	A2	20010612	JP 2000-284780	20000920
EP 1215206	A1	20020619	EP 2000-961096	20000920
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				

PRIORITY APPLN. INFO.: JP 1999-264818 A 19990920
JP 1999-330103 A 19991119
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WO 2000-JP6397 W 20000920

OTHER SOURCE(S): CASREACT 134:252338; MARPAT 134:252338
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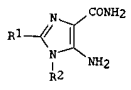
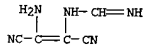


I

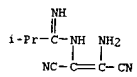
AB The invention provides novel processes for prepg. efficiently compds. of general formula (I) (wherein R1 and R2 are each independently hydrogen, optionally substituted C1-10 alkyl, C3-14 hydrocarbyl bearing an alicyclic skeleton, optionally substituted alkynyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted heterocyclyl, optionally substituted heterocyclylalkyl, N-optionally substituted carbamoyl, or alkoxycarbonyl) and intermediates thereof. Compds. of general formula I can be prepd. by subjecting compds. of general formula R2NHC(R1):NC(CN):C(NH2)CN (II; R1 and R2 are defined above) and/or salts thereof to cyclization hydrolysis in an aq. basic soln. Further, compds. of general formula II can be prepd. from industrially easily available diaminomaleonitrile in a high yield. The compds. I are useful as intermediates for agrochems. and drugs, e.g. dacarbazine and temozoromide (anticancer agent) and urazamide (liver-protective agent). Thus, 50 mL H2O and 43.0 g 25% NaOH were added to 8.0 g N-(2-amino-1,2-dicyanovinyl)formamidine and refluxed for 2 h, cooled to room temp., neutralized with 35% HCl to pH 7, concd. to dryness, treated with ethanol, and filtered for removing the insol. salt. The filtrate was treated with activated charcoal, filtered, and concd. to give a soln. of 4(5)-aminoimidazole-5-carboxamide (III) which was adjusted to pH .ltoreq.3 and cooled at .ltoreq.10.degree.. The pptd. crystals were collected by filtration and dried to give 84% III.HCl.

IT **331282-40-7P**, N-(2-Amino-1,2-dicyanovinyl)formamidine
331282-41-8P, N-(2-Amino-1,2-dicyanovinyl)isobutyramidine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

RN 331282-40-7 CAPLUS
CN Methanimidamide, N-(2-amino-1,2-dicyanoethenyl)- (9CI) (CA INDEX NAME)



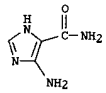
RN 331282-41-8 CAPLUS
CN Propanimidamide, N-(2-amino-1,2-dicyanoethenyl)-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

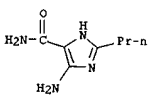
IT **72-40-2P**, 4-Aminoimidazole-5-carboxamide hydrochloride
90521-73-6P, 5-Amino-2-propyl-1H-imidazole-4-carboxamide
227078-19-5P, 5-Amino-2-isopropyl-1H-imidazole-4-carboxamide
331282-42-9P, N-(2-Amino-1,2-dicyanovinyl)butyramidine hydrochloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of aminocarboxamidoimidazoles as intermediates for anticancer and liver-protective agents by cyclization of (aminodicyanovinyl)formamidine derivs.)

RN 72-40-2 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-, monohydrochloride (9CI) (CA INDEX NAME)

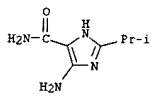


● HCl

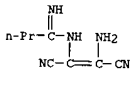
RN 90521-73-6 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-2-propyl- (9CI) (CA INDEX NAME)



RN 227078-19-5 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-2-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 331282-42-9 CAPLUS
CN Butanimidamide, N-(2-amino-1,2-dicyanoethenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

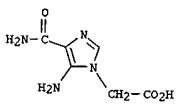
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:270332 CAPLUS
DOCUMENT NUMBER: 133:85826
TITLE: Peptide nucleic acids rather than RNA may have been the first genetic molecule
AUTHOR(S): Nelson, Kevin E.; Levy, Matthew; Miller, Stanley L.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA, 92093-0506, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2000), 97(8), 3868-3871
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Numerous problems exist with the current thinking of RNA as the first genetic material. No plausible prebiotic processes have yet been demonstrated to produce the nucleosides or nucleotides or for efficient two-way nonenzymic replication. Peptide nucleic acid (PNA) is a promising precursor to RNA, consisting of N-(2-aminoethyl)glycine (AEG) and the adenine, uracil, guanine, and cytosine-N-acetic acids. However, PNA has not yet been demonstrated to be prebiotic. We show here that AEG is produced directly in elec. discharge reactions from CH4, N2, NH3, and H2O. Elec. discharges also produce ethylenediamine, as do NH4CN polymns. AEG is produced from the robust Strecker synthesis with ethylenediamine. The NH4CN polymn. in the presence of glycine leads to the adenine and guanine-N9-acetic acids, and the cytosine and uracil-N1-acetic acids are produced in high yield from the reaction of cyanoacetaldehyde with hydantoic acid, rather than urea. Preliminary expts. suggest that AEG may polymerize rapidly at 100.degree. to give the polypeptide backbone of PNA. The ease of synthesis of the components of PNA and possibility of polymn. of AEG reinforce the possibility that PNA may have been the first genetic material.

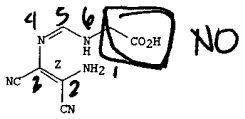
IT **112630-45-2P 281676-74-2P**
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(role of PNA in prebiotic mol. evolution)
RN 112630-45-2 CAPLUS

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)
CN 1H-Imidazole-1-acetic acid, 5-amino-4-(aminocarbonyl)- (9CI) (CA INDEX NAME)



RN 281676-74-2 CAPLUS
CN Glycine, N-{[[(1Z)-2-amino-1,2-dicyanoethenyl]amino]methylene}- (9CI) (CA INDEX NAME)

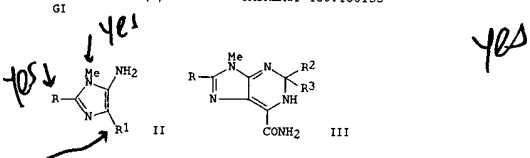
Double bond geometry as shown.



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

submitted in IDS

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:150133 CAPLUS
DOCUMENT NUMBER: 108:150133
TITLE: Chemistry of nitrilium salts. Part 4. Some reactions of 5-amino-4-(C-cyanoformimidoyl)imidazoles obtained from nitrilium trifluoromethanesulfonate salts and diaminomaleonitrile
AUTHOR(S): Booth, Brian L.; Coster, Ronald D.; Fernanda, M.; Proenca, J. R. P.
CORPORATE SOURCE: Inst. Sci. Technol., Univ. Manchester, Manchester, M60 1QD, UK
SOURCE: J. Chem. Soc., Perkin Trans. 1 (1987), (7), 1521-6
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:150133
GI



II III

AB Diaminomaleonitrile reacted readily with RC.tplbond.N+Me O3-SCF3 (R = Me, Ph) to give MeNHC+RNHC(CN):C(CN)NH2 O3-SCF3 (I; R = Me, Ph), which on base treatment under different conditions gave imidazoles II [R1 = cyano, CONH2, C(CN):NH]. I reacted with aldehydes and ketones at room temp. to give trifluorometanesulfonate salts of dihydropurines III [R = Me, Ph; R2 = Me, H; R3 = Me, Ph; R2R3 = (CH2)4]. Similarly II [R = Me, R1 = C(CN):NH] reacted with aldehydes, ketones, 1,2- and 1,3-diketones and keto esters to give dihydropurines III (R = R2 = Me, R3 = Me, Et, Ph, COMe, CH2CO2Et, CO2Et, CH2COMe; R = Me, R2 = Ph, R3 = H, Bz) some of which oxidized in air to purines.

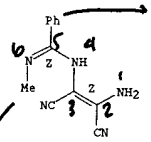
IT **112995-31-0P 112995-33-2P 112995-35-4P 113684-62-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of, with aldehydes and ketones, purines from)
RN 112995-31-0 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,Z)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylbenzenecarboximidamide (1:1) (9CI) (CA INDEX

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)
NAME)

CM 1

CRN 112995-30-9
CMF C12 H11 N5

Double bond geometry as shown.



R_1 = aryl group ⟩ yes.

R_2 = alkyl

CM 2

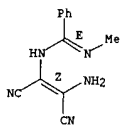
CRN 1493-13-6
CMF C H F3 O3 S

RN 112995-33-2 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,E)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylbenzenecarboximidamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112995-32-1
CMF C12 H11 N5

Double bond geometry as shown.



L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)

CM 2

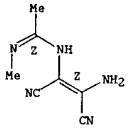
CRN 1493-13-6
CMF C H F3 O3 S

RN 112995-35-4 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,Z)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylethanimidamide (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112995-34-3
CMF C7 H9 N5

Double bond geometry as shown.



CM 2

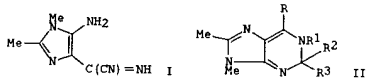
CRN 1493-13-6
CMF C H F3 O3 S

RN 113684-62-1 CAPLUS
CN Methanesulfonic acid, trifluoro-, compd. with (Z,E)-N-(2-amino-1,2-dicyanoethenyl)-N'-methylethanimidamide (1:1) (9CI) (CA INDEX NAME)

CM 1

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1982:19863 CAPLUS
DOCUMENT NUMBER: 96:19863
TITLE: Synthesis of 6-cyano- and 6-carbamoylpurines and 6-carbamoyl-1,2-dihydropurines from N-methylacetonitrilium trifluoromethanesulfonate and diaminomaleonitrile
AUTHOR(S): Booth, Brian L.; Proenca, M. Fernanda
CORPORATE SOURCE: Dep. Chem., Univ. Manchester Inst. Sci. Technol., Manchester, M60 1QD, UK
SOURCE: J. Chem. Soc., Chem. Commun. (1981), (15), 788-9
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB NCC(NH2):C(NH2)CN reacted with [MeC.tplbond.NMe]+ -O3SCF3 to give, after controlled basification (pH 8-9, Na2CO3), 80% imidazole I, which forms 6-cyanopurines with carboxylic acid anhydrides, and with aldehydes, ketones, 1,2- and 1,3-diketones, and keto esters gives 6-carbamoyl-1,2-dihydropurine derivs. from which 6-carbamoylpurines can be obtained. Thus, I with Ac2O gave 80% purine II (R = CN, R1R2 = bond, R3 = Me), whereas I with MeCOCH2CO2Et gave 80% II (R = CONH2, R1 = H, R2 = CH2CO2Et, R3 = Me) which on standing in CHCl3 or EtOH (20.degree., 1-2 days) gave 73% II (R = CONH2, R1R2 = bond, R3 = Me).

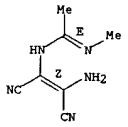
IT **80052-78-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization of)
RN 80052-78-4 CAPLUS
CN Ethanimidamide, N-(2-amino-1,2-dicyanoethenyl)-N'-methyl-, conjugate monoacid, (Z,?)- (9CI) (CA INDEX NAME)

Double bond geometry as described by E or Z.

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)

CRN 113684-61-0
CMF C7 H9 N5

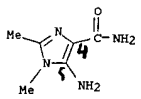
Double bond geometry as shown.



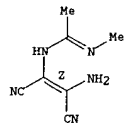
CM 2

CRN 1493-13-6
CMF C H F3 O3 S

IT **78750-93-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 78750-93-3 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-1,2-dimethyl- (9CI) (CA INDEX NAME)

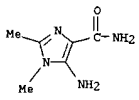


L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS (Continued)



● H+

IT **78750-93-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 78750-93-3 CAPLUS
CN 1H-Imidazole-4-carboxamide, 5-amino-1,2-dimethyl- (9CI) (CA INDEX NAME)



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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	17.95	299.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.48	-2.48

STN INTERNATIONAL LOGOFF AT 16:00:17 ON 16 OCT 2002